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Search for new resonances decaying to pairs of merged diphotons in proton-proton collisions at $\sqrt{s} = 13\,\text{TeV}$

The CMS Collaboration*

Abstract

A search is presented for an extended Higgs sector with two new particles, X and ϕ, in the process $X \to \phi\phi \to (\gamma\gamma)(\gamma\gamma)$. Novel neural networks classify events with diphotons that are merged and determine the diphoton masses. The search uses LHC proton-proton collision data at $\sqrt{s} = 13\,\text{TeV}$ collected with the CMS detector, corresponding to an integrated luminosity of $138\,\text{fb}^{-1}$. No evidence of such resonances is seen. Upper limits are set on the production cross section versus the resonance masses, representing the most sensitive search in this channel.

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*See Appendix A for the list of collaboration members

Many theories of particle physics beyond the standard model (BSM) predict the existence of extended Higgs sectors [1–7]. Such extensions may include an approximate global symmetry with spontaneous symmetry breaking, which is a sufficient condition for the existence of new spin-0 particles, X and ϕ, with unknown masses m_X and m_ϕ. As long as $m_X > 2m_\phi$, $X \to \phi\phi$ is an allowed decay mode, and the ϕ boson can couple to pairs of standard model (SM) particles. The CMS Collaboration previously performed a search targeting $X \to \phi\phi$, considering $\phi \to b\bar{b}$ decays for ϕ boson masses above 25 GeV [8]. Analogously to diphoton decays of the Higgs boson, the ϕ boson can decay to pairs of photons, $\phi \to \gamma\gamma$, via loops of SM or BSM particles [9]. Furthermore, while the ϕ boson may not be massive enough to decay to pairs of heavier fermions, the diphoton decay is particularly important when searching for ϕ bosons with masses below twice the b quark mass. Thus the $\phi \to \gamma\gamma$ channel provides sensitivity in the region of X and ϕ mass combinations that were beyond the reach of the $X \to \phi\phi \to (b\bar{b})(b\bar{b})$ search described in Ref. [8], including the region where the $(b\bar{b})(b\bar{b})$ channel is kinematically allowed but not well reconstructed. Prior searches for similar new spin-0 particles decaying to two photons were performed by the ATLAS Collaboration [10–12]. Searches for exotic decays of the Higgs boson have been performed by the CMS Collaboration; Ref. [13] searched for a four-photon final state and Ref. [14] investigated the regime in which extremely collimated photon pairs are reconstructed as a single photon by the standard CMS algorithm.

This letter presents a search for the production of an X boson, decaying to a pair of ϕ bosons, that themselves decay to pairs of photons, $X \to \phi\phi \to (\gamma\gamma)(\gamma\gamma)$. The analysis focuses on a broad range of m_X between 0.3 and 3 TeV, with a relative mass $\alpha = m_\phi/m_X$ ranging between 0.5 and 2.5% resulting in Lorentz boosts of the ϕ bosons in the range 14 to 200. These mass combinations correspond precisely to the regime where the previous $\phi \to b\bar{b}$ search has no sensitivity. The Lorentz boost causes the two photons from a ϕ boson decay to be too merged to be individually identified, but not so collimated that the signature would be consistent with a single photon in the standard CMS reconstruction [15]. To gain sensitivity in this intermediate regime, a dedicated convolutional neural network (CNN) has been developed, which classifies energy clusters in the CMS electromagnetic calorimeter (ECAL) as originating from two overlapping photons (denoted Γ), hadronic activity, or a single photon. A second CNN is used to reconstruct the mass of the Γ candidates, similar to [16], optimized for the exploration of the α–m_X space considered in this letter. After selecting events with two Γ candidates, the analysis searches for localized excesses over the steeply falling background distribution of their paired reconstructed mass ($m_{\Gamma\Gamma}$), in slices of the reconstructed mass ratio $\alpha^{\text{reco}} = \hat{m}_\Gamma/m_{\Gamma\Gamma}$, where $\hat{m}_\Gamma$ is the average reconstructed mass of the two Γ candidates. The background in this search is derived exclusively from a parameterized fit to the data.

The search uses a data set of proton-proton (pp) collisions at $\sqrt{s} = 13$ TeV at the CERN LHC, collected with the CMS detector in 2016–2018, corresponding to an integrated luminosity of 138 fb^{-1}. The CMS apparatus [17] is a multipurpose, nearly hermetic detector, designed to trigger on [18, 19] and identify electrons, muons, photons, and hadrons [20–22]. A global reconstruction algorithm [23] combines the information provided by the all-silicon inner tracker and by the lead tungstate ECAL and brass-scintillator hadron calorimeters, operating inside a 3.8 T superconducting solenoid, with data from gas-ionization muon detectors embedded in the solenoid return yoke, to build τ leptons, jets, missing transverse momentum, and other physics objects [24–26]. Events are retained for analysis if they pass a trigger requiring two photon candidates, each with $p_T > 60$ or 70 GeV in 2016 or 2017–2018 data, respectively. The photon identification algorithm used by the trigger only selects photons based on isolation, and not on the cluster shape, and hence has high efficiency for selecting events with two merged diphotons, provided they have sufficient p_T. Tabulated results for this analysis are provided in

the HEPData record [27].

The ECAL barrel covers a pseudorapidity range $|\eta| < 1.4$ and consists of 61,200 individual crystals, each covering $\Delta\eta \times \Delta\phi = 0.0175 \times 0.0175$ where ϕ is the azimuthal angle. Individual photons typically deposit energy in several adjacent crystals, and are reconstructed as localized clusters of energy. For merged diphotons, such clusters may overlap. Purpose-built algorithms for identifying diphotons from the shapes of their energy distributions in the ECAL barrel are described below. To simplify the CNN implementation, this analysis uses events where both Γ candidates are reconstructed in the barrel, which account for more than 60% of the expected signal yield.

The benchmark signal model $X \to \phi\phi \to (\gamma\gamma)(\gamma\gamma)$ is generated at leading order with the MADGRAPH5_aMC@NLO 2.6.0 [28] generator, with up to two additional partons in the matrix element calculations. Simulated signals are generated for m_X from 0.3 to 3 TeV (at intervals ranging from 0.1 to 0.5 TeV) and for α from 0.5 to 2.5% (at 0.5% intervals). The X boson is produced via gluon fusion, and its coupling to gluons is evaluated by integrating over N flavors of new Dirac fermion quarks that receive all their mass from the X vacuum expectation value f, such that the cross section depends only on $(m_X N)/f$, in the limit that the quarks are much heavier than X. The signal production cross section is calculated numerically at next-to-next-to-leading order (NNLO) using the HQT 2.0 program [29–31]. The background from SM production of jets and photons (γ+jets), used to optimize the analysis procedure, is also modeled at next-to-leading order with the MADGRAPH5_aMC@NLO generator. Hadronic objects for training of the classification CNN are taken from this sample. The parton showering and fragmentation for these samples is modeled by PYTHIA 8.240 [32]. Matching between the matrix element and parton shower jets relies on the MLM matching procedure [33]. Samples of isolated photons and diphotons with uniform energy distributions are generated with PYTHIA 8.107 [34] and are used to train the Γ identification and mass reconstruction CNNs. The CP5 [35, 36] underlying event tune is used for the simulation with the NNPDF3.1 [37] NNLO parton distribution function sets. The response of the CMS detector is modeled using GEANT4 [38]. The effect of extra pp interactions in the same or adjacent bunch crossings (pileup) is incorporated in the simulation, with the frequency distribution of additional vertices adjusted to match that observed in data.

Energy deposits in the ECAL barrel are clustered into Γ candidates using an algorithm inspired by the Cambridge–Aachen algorithm [39]. Beginning with the most energetic single-crystal deposit in the ECAL barrel, the nearest neighbor energy deposit is iteratively added to the cluster if the ΔR between the deposit and the energy-weighted average position of the current cluster is less than a radius $R = 0.15$, where $\Delta R = \sqrt{\Delta\eta^2 + \Delta\phi^2}$. When no new crystals can be included in a cluster, the process begins again with the highest energy unclustered deposit. The distance parameter was chosen to be large enough to capture both photons from a single ϕ boson decay in a single cluster, but not so large that the usual CMS photon identification would reconstruct two separate photons. For the range of α values considered in this analysis, the simulated efficiency of this algorithm to capture both photons in the cluster ranges from 80–100%, while the efficiency of requiring two individually identified photons ranges from $\sim$1 to 20%.

Each Γ candidate consists of a collection of energy deposits on an array of crystals, and can be represented as a pixelated image. Convolutional neural networks developed for image recognition are well suited to extract relevant information about the Γ candidates. The clustered energy deposits are converted to a 30×30 image, centered on the most energetic deposit, where the brightness of a pixel corresponds to the energy deposited in a single crystal. Two different

CNNs are used. The first separates Γ candidates arising from merged diphotons from those produced by hadronic decays and single photons. The second regresses the mass-to-energy ratio (m/E) of the Γ candidate, under the assumption that it was produced by a genuine diphoton. The architectures of both CNNs are based on the DEEPTOP [40] CNN, modified as described below.

For both CNNs, the inputs are the individual crystal energies of that Γ candidate, normalized such that the sum of all crystal energies is unity. These are passed through a series of four convolutional layers with kernels of sizes 7×7, 5×5, 4×4, and 3×3, with 64 output feature maps after each layer in the classification network and 16 in the mass regression network. For the classification, this is followed by one fully-connected (FC) linear layer with three outputs corresponding to the output classes. A logarithmic softmax function is used to convert these to probabilities that the cluster belongs to each category: diphoton ($P_{\gamma\gamma}$), photon (P_{γ}), or hadron (P_{had}). For the mass regression, three FC layers are used with output sizes of 64, 16, and 1, respectively, and the geometric η of the Γ candidate is used as an additional input to the first FC layer. The output of the regression CNN is a single number corresponding to the predicted value of m/E.

The training of the classification CNN uses 600k events, divided equally between the diphoton, single photon, and hadron categories. For the regression, 500k simulated diphoton events are used. In both cases, diphoton events are sampled to retain a flat m/E spectrum from 0 to 0.07. The loss function used for classification is the categorical cross-entropy function; for the regression, a modified mean squared error function optimized for small positive values is used: $\sum_i -\log\left(\mathrm{e}^{-(p_i-q_i)^2}\right) + \log\left(1-\mathrm{e}^{-(p_i-q_i)^2}\right)$, where p_i, q_i are the true and predicted m/E values for the ith event, respectively.

To suppress the dominant background from misidentified jets, a relative isolation r_{iso} is defined and applied to each Γ candidate in the analysis. Jets reconstructed with the anti-k_{T} algorithm [41] and a distance parameter of 0.4, using the FASTJET package [42], are used. If a Γ candidate overlaps with such a jet within $\Delta R < 0.15$, its r_{iso} is defined as the ratio of its energy to that of the jet. Otherwise, it is set to unity.

The diphoton decays of π^0 or η mesons copiously produced in hadronic showers can be used to validate the performances of the CNNs. While the technique developed in Ref. [16] utilizes π^0 decays to validate its mass regression, here the η meson is used, highlighting the complementarity of the kinematic regions explored. An η meson control sample is selected to validate the efficiency of the signal classification and the scale and resolution of the m/E regression. The control sample is taken from all events passing an electron or photon trigger. The Γ candidates are required to have energies in the range 30–60 GeV and $r_{\text{iso}} > 0.5$. This energy range is selected such that the η meson decay products form a single Γ candidate, covering the Lorentz boost range of the signals considered. The m_{Γ} distributions are compared in two subsets, depending on whether $P_{\gamma\gamma} > 0.9$ or not (referred to as "passing" and "failing" regions). The m_{Γ} distributions of the passing and failing regions are presented in Fig. 1, showing a distinct peak at the η meson mass, providing strong evidence that the regression CNN is working as intended. Due to contamination from other particles produced in the same jet, a substantial number of η mesons decaying to collimated diphotons will appear in the failing region, resulting in the peak seen there. The data and the simulation are each fit simultaneously in the passing and failing regions; the mass of the η meson in both is reconstructed to within 2% of its true value. The classifier efficiency and the mean and width of the peak are extracted using a fit to data, where the signal (background) is modeled by a Gaussian (exponential) function. The classifier efficiency in the η meson control region is measured to be 55 (53)% in data (simu-

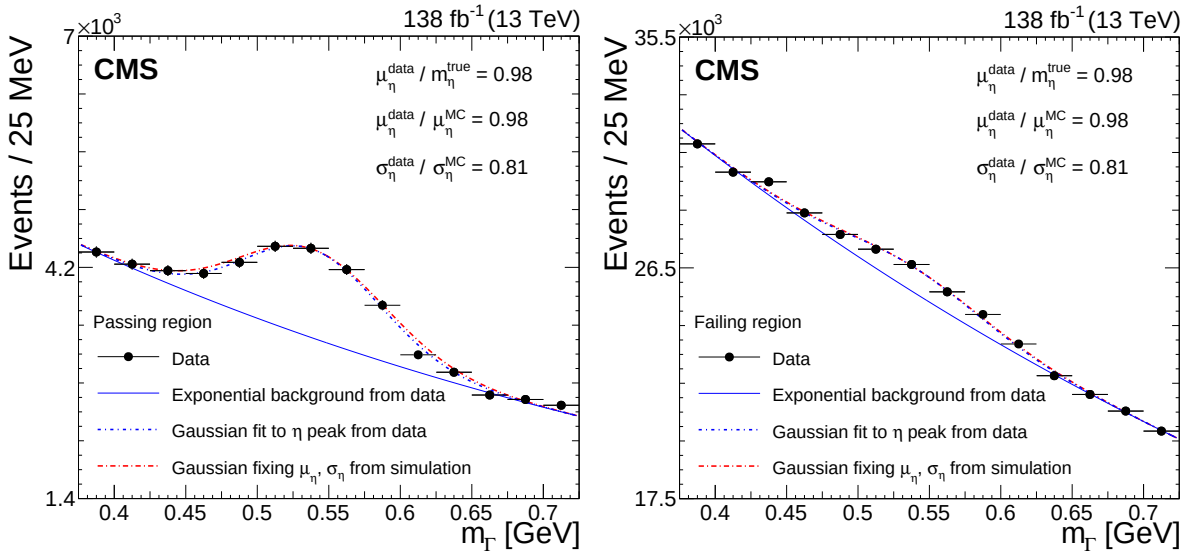

Figure 1: Cluster mass (m_Γ) distribution in data for both the passing (left) and failing (right) regions, in the energy range for which the η meson is expected to form a single Γ candidate. The signal (background) is modeled by a Gaussian (exponential) function. Blue and red dashed lines depict Gaussian fits to the data and Monte Carlo (MC) simulation, respectively. The solid blue line shows the background component of the fit. Ratios of the Gaussian fit means (μ) and widths (σ) are displayed, where m_η^{true} is the true mass of the η meson.

lation). The data-to-simulation efficiency ratio is consistent with unity, with a total uncertainty of 10% that is propagated to the final results. The systematic uncertainty in the m_Γ resolution is obtained from the difference in the widths of the η meson peaks in data and simulation, corresponding to 23%. Finally, the mean positions of the peaks are found to be consistent between data and simulation, and are within the m_Γ resolution uncertainty.

We further validate the performance of the regressor and classifier using a control sample of reconstructed Z bosons through the decay $\mathrm{Z} \to \mathrm{e}^+\mathrm{e}^-$ by exploiting the case when each electron undergoes bremsstrahlung and appears consistent with a merged diphoton signature. Events are selected by requiring two clusters with $P_{\gamma\gamma} > 0.75$ and $r_{\text{iso}} > 0.8$. The resulting reconstructed $m_{\Gamma\Gamma}$ distribution shows a clear presence of Z bosons in both data and simulation, with nearly identical performance. The positions of the reconstructed mass peaks in data and simulation are found to be within 0.5% across a wide range of cluster p_T, and this value is applied as a systematic uncertainty in the Γ candidate energy scale.

The offline analysis considers events with two Γ candidates in the ECAL barrel with $p_\mathrm{T} > 90\,\text{GeV}$, where the trigger becomes fully efficient. Both Γ candidates must also fulfill the following requirements: $r_{\text{iso}} > 0.8$ and $P_{\gamma\gamma} > 0.9$. This $P_{\gamma\gamma}$ requirement retains $\gtrsim$80% of simulated signal across all masses and rejects approximately 99% of the background. The mass asymmetry of the event $m_{\text{asym}} = |m_{\Gamma_1} - m_{\Gamma_2}|/(m_{\Gamma_1} + m_{\Gamma_2}) < 0.25$ is required. Finally, $\eta < 1.5$ (between the candidates) is required to further suppress background from the SM production of jets and photons.

The remaining data are evaluated for localized excesses in the $m_{\Gamma\Gamma}$ distribution, in nine non-overlapping divisions of the α^{reco} distributions ranging from 0.3 to 3%, each determined by a combination of detector resolution and a requirement that the division contains enough events for the background estimate to converge. Any particular signal is expected to appear in only a few adjacent α^{reco} divisions. As in previous searches [43–46], the background differential cross

section ($d\sigma/dm_{\Gamma\Gamma}$) is modeled by fitting empirical functional forms to the observed data in each division, where the number of parameters in the functional forms is determined by performing Fisher F-tests [47] on progressively higher-order functions. Functions with three parameters were found to be optimal for describing the data: the dijet function $p_0(1-x)^{p_1}/x^{p_2}$, the modified dijet function $p_0(1-x^{1/3})^{p_1}/x^{p_2}$, the diphoton function $p_0 x^{p_1+p_2 \log x}$, a power-law times an exponential function $p_0 e^{-p_1 x}/x^{p_2}$, and a four-parameter power-law function $p_0 p_1^{p_2 x+p_3/x}$, where x is $m_{\Gamma\Gamma}/\sqrt{s}$. The choice of function is encoded into the fitting procedure as a discrete parameter of the likelihood. Signal shapes are modeled by fitting a double-sided Crystal Ball function [48] to the reconstructed simulated signal $m_{\Gamma\Gamma}$ spectra, then interpolating the function parameters to generate shapes with fine spacing in m_X. To validate the robustness of the fit, a goodness-of-fit test and bias tests are performed. The bias tests use simulated events with a variety of simulated signals injected. No significant bias is observed for any X and ϕ boson mass combination. The result of the fit for one representative α^{reco} division is shown in Fig. 2. The search uses a fit of the background function plus the simulated signal shape to the data, taking into account statistical and systematic uncertainties, and is performed for $m_{\Gamma\Gamma} > 297\,\text{GeV}$ and simultaneously in all bins of α^{reco}.

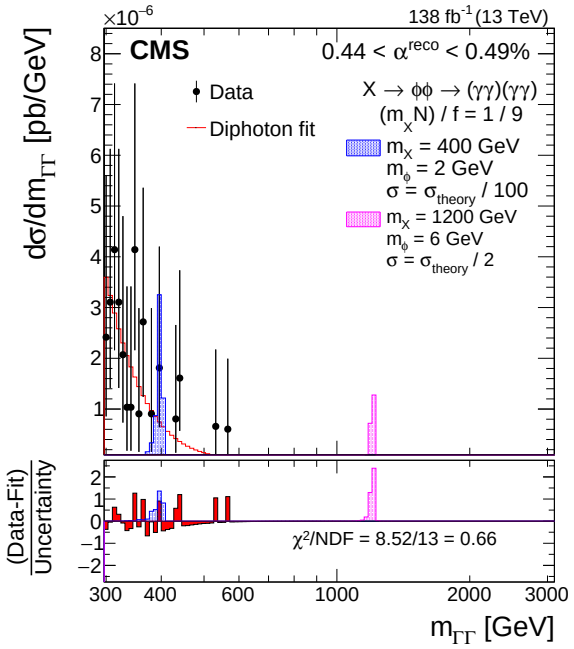

Figure 2: Dicluster mass ($m_{\Gamma\Gamma}$) distribution for the data (points) for one of the α^{reco} bins of the search ($0.44 < \alpha^{\text{reco}} < 0.49\%$), fitted with the diphoton function (red), one of the considered five background parametrizations. Examples of two representative predicted signals are shown (blue and pink). The lower panel shows the difference between the observed data and the background prediction divided by the statistical uncertainty of the data (σ_{data}), the aforementioned signals divided by σ_{data}, and the goodness of fit measure χ^2/NDF (where NDF is the number of degrees of freedom).

Systematic uncertainties are modeled in the fit as nuisance parameters that affect the shapes and normalizations of signal and background processes, with log-normal priors for the uncertainties affecting only the normalization and Gaussian priors for those affecting the shapes of distributions. The main sources of systematic uncertainty in the background modeling are the choice of the background function and the background function fit parameters. The parameters of the background function are treated as freely floating nuisance parameters, and are

evaluated via profiling. The discrete profiling method [49] is used for considering the choice of the functional form as a discrete nuisance parameter, which is profiled in an analogous way to continuous nuisance parameters. Systematic uncertainties affecting the predicted signal yield include the uncertainty in the integrated luminosity measurement (1.6%) [50–52], the diphoton classifier efficiency (10%, applied per cluster), the m_Γ resolution uncertainty (23%, affecting the yield in each α^{reco} bin), and the trigger efficiency (5%). Systematic uncertainties affecting the shape of the predicted signal distributions include the Γ energy scale uncertainty (0.5%, applied per cluster) and uncertainties in the modeling of pileup (1–10%). The dominant systematic uncertainty in the signal modeling is due to the diphoton classifier efficiency.

No significant excesses compatible with the signal hypotheses are observed. The largest excess corresponds to $m_X \approx 720\,\text{GeV}$ and $\alpha = 0.7\%$ ($m_\phi \approx 5\,\text{GeV}$) with a local (global) significance of 3.57 (1.07) standard deviations. The global significance accounts for the look-elsewhere effect [53] by using pseudo-experiments to compute the probability that the background hypothesis produces a signal-like fluctuation with at least the observed local significance anywhere in the sensitive range of m_X and α. The fit results are used to set 95% confidence level (CL) upper limits on the cross section $\sigma(\text{pp} \to \text{X})$, assuming a 100% branching fraction for $\text{X} \to \phi\phi \to (\gamma\gamma)(\gamma\gamma)$. Upper limits are computed using a modified frequentist approach, based on the CL_s criterion [54–56], with the profile likelihood ratio used as the test statistic within the asymptotic approximation [57]. Observed and expected limits are computed as functions of m_X for a given true value of α, and compared to the theoretical estimates of $\sigma(\text{X} \to \phi\phi)$ for a set of $(m_X N)/f$ values. Figure 3 shows the observed upper limits on the cross section and the mass exclusion curves in the α–m_X plane. The observed (expected) upper limits on this process range from 0.03–1.06 (0.03–0.79) fb, depending on m_X and m_ϕ.

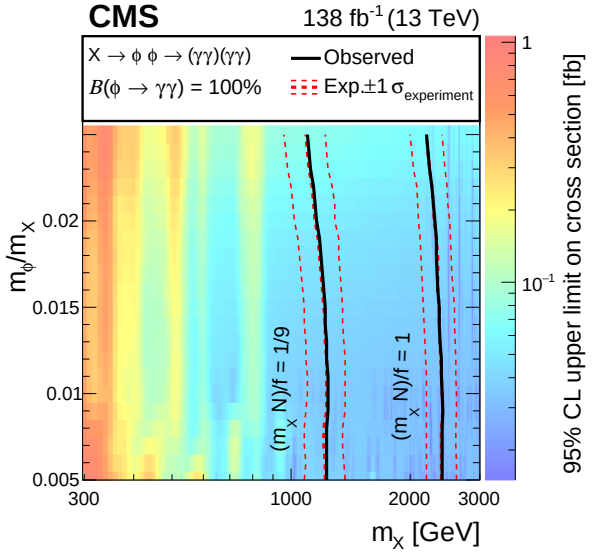

Figure 3: Exclusion limits at 95% CL on $\sigma(\text{X} \to \phi\phi \to (\gamma\gamma)(\gamma\gamma))$ displayed in the (m_ϕ/m_X)–m_X plane. Branching fractions ($\mathcal{B}$) of both $\text{X} \to \phi\phi$ and $\phi \to \gamma\gamma$ are assumed to be 100%. The black (red) lines represent the observed (expected) mass exclusions corresponding to different assumptions of $(m_X N)/f$. The observed upper limits on the cross section are shown on the color z axis.

In summary, a search for an extended Higgs sector with two new particles, X and ϕ, with unknown masses m_X and m_ϕ, has been presented for the decay sequence $\text{X} \to \phi\phi \to (\gamma\gamma)(\gamma\gamma)$. The search uses proton-proton collision data at $\sqrt{s} = 13\,\text{TeV}$, collected with the CMS detector at the LHC in 2016–2018, corresponding to an integrated luminosity of $138\,\text{fb}^{-1}$. The analysis

considers m_X between 0.3 and 3 TeV, and is restricted to values of m_ϕ for which the ratio m_ϕ / m_X is between 0.5 and 2.5%. As a result, the two photons from each ϕ boson overlap significantly in the electromagnetic calorimeter. Convolutional neural networks trained on clusters of calorimeter energy deposits are used to classify events containing merged diphotons and to regress the mass of the diphoton system. The dicluster mass spectra, in bins of the ratio of the average cluster mass divided by the dicluster mass, are analyzed for the presence of new resonances, and are found to be consistent with the standard model expectations. Upper limits are set at 95% confidence level (CL) on the production cross section for $X \to \phi\phi \to (\gamma\gamma)(\gamma\gamma)$, as a function of the resonance masses, where both the $X \to \phi\phi$ and $\phi \to \gamma\gamma$ branching fractions are assumed to be 100%. Observed (expected) limits range within 0.03–1.06 (0.03–0.79) fb at 95% CL for the masses considered. These results represent the most sensitive search of an extended Higgs sector with this final state.

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